Amendments to the Claims:

This listing of claims replaces all prior versions and listings of claims in the application.

Listing of Claims:

1. – 36. (Cancelled).

37. (**Currently amended**) A machine having a processor and a ~~memory~~ data storage medium, the processor communicatively coupled to the ~~memory~~ data storage medium, and the ~~memory holding~~ data storage medium storing instructions for performing a method comprising:

receiving information relating to a monoatomic metal ion to be simulated;

and generating, for observation by a user on a display, a representation of ~~a~~ the monoatomic metal ion as a metal molecule by a molecular dynamics simulation, wherein said ~~representation of a metal ion~~ metal molecule comprises a plurality of atoms comprising a center atom and one or more dummy atoms, wherein said center atom has ~~having~~ a van der Waals radius greater than zero, wherein said center atom is covalently linked to said one or more dummy atoms, and wherein each dummy atom ~~having~~ has a positive charge.

38. (Previously Presented) The machine of claim 37 wherein said dummy atom has a mass of about 0.1 g/mol.

39. (Previously Presented) The machine of claim 37 wherein said dummy atom has a mass greater than about 0.1 g/mol.

40. (Previously Presented) The machine of claim 37 wherein said dummy atoms are located at the apices of a polyhedron.

41. (Previously Presented) The machine of claim 40 wherein said center atom is located at the center of said polyhedron.

42. (Previously Presented) The machine of claim 40 wherein said polyhedron is selected from the group consisting of tetrahedron, trigonal bipyramid, square pyramid, and octahedron.

43. (Previously Presented) The machine of claim 41 wherein said polyhedron is a tetrahedron.

44. (Previously Presented) The machine of claim 37 wherein said metal ion is selected from a main group metal or transition metal.

45. (Previously Presented) The machine of claim 37 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.

46. (Previously Presented) The machine of claim 37 wherein said metal ion is zinc.

47. (Previously Presented) The machine of claim 41 wherein said metal ion is zinc.

48. (Previously Presented) The machine of claim 37 wherein said metal ion is magnesium.

49. (Previously Presented) The machine of claim 37 wherein said metal ion is calcium.

50. (Previously Presented) The machine of claim 37 wherein said metal ion has a calculated energy of solvation about equal to an experimentally determined energy of solvation for said metal ion.

51. (Previously Presented) The machine of claim 50 wherein said calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.

52. (Previously Presented) The machine of claim 37 wherein said dummy atom has a charge of about + 0.5.

53. (Previously Presented) The machine of claim 37 wherein said dummy atom has a charge of about + 0.3333.

54. (Previously Presented) The machine of claim 37 wherein said dummy atom has a charge ranging from about +0.1 to about +3.

55. (**Currently amended**) A computer readable medium having computer executable instructions stored thereon, wherein the execution of said instructions simulates a monoatomic metal ion as a metal molecule for observation by a user on a display, said metal molecule comprising a plurality of atoms comprising a center atom and one or more dummy atoms, wherein said center atom has ~~having~~ a van der Waals radius greater than zero, wherein said center atom is covalently linked to said one or more dummy atoms, and wherein each dummy atom ~~having~~ has a positive charge.

56. (Previously Presented) The computer readable medium of claim 55 wherein said dummy atom has a mass of about 0.1 g/mol.

57. (Previously Presented) The computer readable medium of claim 55 wherein said dummy atom has a mass greater than about 0.1 g/mol.

58. (Previously Presented) The computer readable medium of claim 55 wherein said dummy atoms are located at the apices of a polyhedron.

59. (Previously Presented) The computer readable medium of claim 58 wherein said center atom is located at the center of said polyhedron.

60. (Previously Presented) The computer readable medium of claim 58 wherein said polyhedron is selected from the group consisting of tetrahedron, trigonal bipyramid, square pyramid, and octahedron.

61. (Previously Presented) The computer readable medium of claim 59 wherein said polyhedron is a tetrahedron.

62. (Previously Presented) The computer readable medium of claim 55 wherein said metal ion is selected from a main group metal or transition metal.

63. (Previously Presented) The computer readable medium of claim 55 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.

64. (Previously Presented) The computer readable medium of claim 55 wherein said metal ion is zinc.

65. (Previously Presented) The computer readable medium of claim 59 wherein said metal ion is zinc.

66. (Previously Presented) The computer readable medium of claim 55 wherein said metal ion is magnesium.

67. (Previously Presented) The computer readable medium of claim 55 wherein said metal ion is calcium.

68. (Previously Presented) The computer readable medium of claim 55 wherein said metal ion has a calculated energy of solvation about equal to an experimentally determined energy of solvation for said metal ion.

69. (Previously Presented) The computer readable medium of claim 68 wherein said calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.

70. (Previously Presented) The computer readable medium of claim 55 wherein said dummy atom has a charge of about + 0.5.

71. (Previously Presented) The computer readable medium of claim 55 wherein said dummy atom has a charge of about + 0.3333.

72. (Previously Presented) The computer readable medium of claim 55 wherein said dummy atom has a charge ranging from about +0.1 to about +3.